

## Resistance-Distance Sum Rules\*

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The chemical potential for a novel intrinsic graph metric, the resistance distance, is briefly recalled, and then a number of »sum rules« for this metric are established. »Global« and »local« types of sum rules are identified. The sums in the »global« sum rules are graph invariants, and the sum rules provide inter-relations amongst different invariants, some involving the resistance distance while others do not. Illustrative applications to more »regular« graphs are made.

*Key words:* resistance distance, connectivity index, regular polyhedra.

### INTRODUCTION

A novel distance function on a graph was identified<sup>1</sup> a few years back. And though this »resistance distance« function appearing as part of electrical circuit theory had been intensively studied in physics, in engineering, and in mathematics, it rather amazingly apparently had been without recognition that it is a distance function (or metric) on graphs. For instance, it is not mentioned in Buckley and Harary's<sup>2</sup> monograph on *Distances in Graphs*. The term *resistance distance* was used because of the physical interpretation: one imagines unit resistors on each edge of a graph  $G$  and takes the resistance distance between vertices  $i$  and  $j$  of  $G$  to be the effective resistance between vertices  $i$  and  $j$  (as when a battery is attached at these two vertices). This resistance distance is in fact intrinsic to the graph, with

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\* Dedicated to the Professor Milan Randić on the occasion of his 70th birthday.

some nice purely mathematical interpretations also, as reviewed in Refs. 3 and 4, though three of these alternate interpretations were earlier established before recognition of the function as a metric. On the other hand there is the long recognized »shortest-path« distance function which has been extensively studied.<sup>2</sup> In fact the resistance and shortest-path distances agree whenever in the graph there is but one path between the two considered vertices – and otherwise the resistance distance becomes diminished from this reference when there are multiple pathways between the two vertices (regardless of whether the two distinct paths are disjoint or not). That is multiple pathways between two vertices not unsurprisingly engender better »communication« with a consequent lessening of the effective distance (or resistance) between the two vertices. As such, the shortest-path distance might be imagined to be more relevant when there is corpuscular communication (along edges) between two vertices, whereas the resistance distance might be imagined to be more relevant when the communication is wave- or fluid-like. Thence concerning electronic wave-functions one naturally imagines the relevance of the resistance distance. Indeed paying attention to multiple pathways between a pair of vertices is of paramount importance even in classical chemistry, as witnessed by the importance of distinguishing between single and double (or triple) bonds, and in the relevance of 6-cycles in organic aromatics. But so far there has been only preliminary chemical application (*e.g.*, as Refs. 5–7) of the resistance distance, but that chemical communication in molecules is rather wave-like suggests the utility of the concept. Of course there are multifarious applications in physics and electrical engineering, but evidently they have been (rather successfully) pursued without explicit use of the metricity of the concept (of electrical resistance). Even Snelling and Doyle's<sup>8</sup> charming mathematically oriented book (which incidently emphasizes a nice probabilistic interpretation of the resistance between two vertices) does not identify this as a metric.

At present it seems that the development of further methodologies and theorems concerning such a fundamental concept (with a substantial potential for chemical applications, beyond the traditional electrical ones) may be of interest. This is the broad aim here. In particular an extension is sought of some earlier work<sup>1</sup> involving a broad class of formulas for selected sums of resistance distances. The theoretical development of such »sum rules« is described in the section Mathematical Formulation and Results for General Graphs, with some attempt at the identification of systematic sets of such sum rules. Thereafter in the section Specialized Results for Highly Regular Graphs we indicate substantial simplifications which occur with more regular graphs, it being noted that some resistance distances between closer sites may sometimes be especially simply determined, and a few illustrative applications are made.

# MATHEMATICAL FORMULATION AND RESULTS FOR GENERAL GRAPHS

Standard notation for a (molecular) graph  $G$  is used. The vertex (or site) set is  $V$  and the edge (or bond) set is  $E$ . Resistance distances are neatly given in terms of a graph's so-called Laplacian matrix. This matrix  $L$  has rows and columns labelled by the vertices of the graph  $G$ , so that if  $N$  is the number of sites, the matrix is  $N \times N$ , and  $L$  may be expressed as a difference  $L \equiv \Delta - A$  between the diagonal matrix  $\Delta$  of site degrees and the usual adjacency matrix  $A$ . That is, the elements  $\Delta_{ij}$  are 0, except for the  $(i = j)$  diagonal for which  $\Delta_{ii}$  is the degree  $\Delta_i$  of site  $i \in V$ , and the elements  $A_{ij}$  are 0 except for  $i, j$  which are adjacent (in  $G$ ) whence  $A_{ij} = 1$ . The matrix  $L$  may be viewed as a sort of discretized representation of the Laplacian operator of conventional analysis and mathematical physics, and so may naturally be expected to be of a fundamental nature in graph theory. And indeed it has been much studied, *e.g.*, as reviewed in Refs. 9–11.

For a *connected* graph  $G$  as are the subject of study here, it may be readily seen that  $L$  has all eigenvalues positive except one that is 0. The eigenvector  $\phi$  associated to this 0-eigenvalue has all its components the same, which we might take to be 1. Then  $L$  has a generalized inverse  $\Gamma$ , which has  $\phi$  as a 0-eigenvalue eigenvector, and on the space orthogonal to  $\phi$ ,  $\Gamma$  is the ordinary inverse to  $L$  restricted to this same space. The matrix  $\Phi$  with all its elements being  $1/N$  is a projection operator  $\Phi = N^{-1}\phi\phi^\dagger$ . If  $I$  denotes the identity matrix, then

$$L\Gamma = \Gamma L = I - \Phi$$

this resultant being essentially the full  $N$ -dimensional space extension of the identity matrix for the subspace orthogonal to  $\phi$ . And there is a fundamental result that the resistance  $\Omega_{ij}$  between two vertices  $i$  and  $j$  of  $G$  is given in terms of the elements of  $\Gamma$  by

*Theorem A* – Let a connected graph  $G$  have Laplacian matrix  $L$ , and let its generalized inverse (as above) be  $\Gamma$ . Then the resistance distance between vertices  $i$  and  $j$  of  $G$  is

$$\Omega_{ij} = \Gamma_{ii} - \Gamma_{ij} - \Gamma_{ji} + \Gamma_{jj}$$

and this is a metric on the graph.

The formula of this theorem may be formally derived<sup>1</sup> using Kirchoff's laws, and seems to have been long known in the electrical engineering literature, with it appearing in several texts, such as Ref. 12. For our present

purposes the formula of this theorem might just be accepted as a definition of the resistance distance.

One of the various consequences of this result is:

*Theorem B* – For  $G$  an  $N$ -site connected graph and an arbitrary  $N \times N$  matrix  $M$ ,

$$\sum_{i,j \in V} (LML)_{ij} \Omega_{ij} = -2 \operatorname{tr}\{ML\}$$

(Here  $\operatorname{tr}$  denotes the trace operation, which sums over the diagonal elements of the matrix argument.) A proof is found in Ref. 1, but may be established here again. One merely substitutes the result of theorem A into the left-hand side of the present formula to obtain

$$\sum_{i,j \in V} (LML)_{ij} (\Gamma_{ii} - \Gamma_{ij} - \Gamma_{ji} + \Gamma_{jj}) = 2 \sum_{i,j \in V} \Gamma_{ii} (LML)_{ij} \varphi_j - 2 \sum_{i \in V} (LML\Gamma)_{ii}$$

where we have used the symmetry of the matrices, and introduced the elements  $\varphi_i = 1$  of the special vector  $\varphi$ . Because  $\varphi$  is a 0-eigenvalue eigenvector to  $L$ , the first summation here vanishes, and in the second the product  $L\Gamma$  may be replaced by  $I - \Phi$ , to obtain

$$0 - 2 \sum_{i \in V} (LM(I - \Phi))_{ii} = -2 \sum_{i \in V} (LM)_{ii} - 0 = -2 \operatorname{tr}(LM)$$

and thereby establish the theorem.

This theorem B may be viewed as a general »sum rule« for resistance distances, with different particular realizations for different particular choices of  $M$ . For the case of  $M = \Gamma$  one is fairly directly led to

*Corollary C* – For  $G$  an  $N$ -site connected graph with edge set  $E$ ,

$$\sum_{\{i,j\} \in E} \Omega_{ij} = N-1 .$$

In fact this particular result was long ago established by Foster<sup>13</sup> and by Weinberg.<sup>14</sup>

Ref. 1 goes on to consider a couple other sum rules specialized to the case of highly regular graphs, but here we first consider the case of general connected graphs. The first type are »global« and lead to relations amongst graph invariants, whereas the second type are »local« and entail relations amongst different subsets of sites in one or more local regions of the parent graph. Such »local« subsets of sites might for instance be those of the *neighbor* set  $n(a)$  of a given site  $a \in V$ . These »local« sum rules arise with a »local« choice for the matrix  $M$  in theorem B, but there is a great deal of latitude in

choosing  $\mathbf{M}$  – all that is required is that it be of the proper dimension ( $N \times N$ ). A candidate for a canonical set of local sum rules is:

*Theorem D* – Let  $a, b \in V$  in a connected graph  $G$ . Then

$$\Delta_a^{-1} \sum_{i,j \in n(a)} \Omega_{ij} = \sum_{i \in n(a)} \Omega_{ia} - 1$$

$$\Delta_a \Delta_b \Omega_{ab} - \Delta_a \sum_{j \in n(b)} \Omega_{aj} - \Delta_b \sum_{i \in n(a)} \Omega_{ib} + \sum_{i \in n(a)} \sum_{j \in n(b)} \Omega_{ij} = 2\delta_{a \sim b}, \quad a \neq b$$

where  $\delta_{a \sim b}$  is 0 unless  $a$  and  $b$  are neighbors in which case it takes the value 1.

The proof proceeds from theorem *B* with the choice of  $\mathbf{M}$  as the matrix  $\mathbf{O}_{ab}$  which has all elements 0 except the  $(a, b)$ th element which is 1. The  $b = a$  choice  $\mathbf{M} = \mathbf{O}_{aa}$  leads to the first consequence of the theorem (when it is also recalled that  $\mathbf{L} = \Delta - \mathbf{A}$ ). The choice of  $\mathbf{M} = \mathbf{O}_{ab}$  with  $b \neq a$  leads to the second consequence of the theorem.

This theorem *D* provides a hierarchy of conditions each correlating with a pair of vertices  $a, b$ . In fact it can be shown that the conditions of this theorem in essence determine all the  $\Omega_{ij}$ .

*Theorem E* – For a connected graph  $G$ , the conditions of theorem *D* determine all the  $\Omega_{ij}$ , if also it is understood that  $\Omega_{ij} = \Omega_{ji}$  and  $\Omega_{ii} = 0$ , all  $i, j \in V$ .

A proof begins with a recasting of the conditions of theorem *D* into a suitably compact form, namely as

$$\sum_{i,j \in V} (\mathbf{L} \otimes \mathbf{L})_{ab,ij} \Omega_{ij} = 2\mathbf{L}_{ab}$$

where  $\mathbf{B} \otimes \mathbf{C}$  denotes the ( $N^2 \times N^2$ ) Kronecker product of two ( $N \times N$ ) matrices  $\mathbf{B}$  and  $\mathbf{C}$ , with the elements of  $\mathbf{B} \otimes \mathbf{C}$  given by  $(\mathbf{B} \otimes \mathbf{C})_{ab,ij} \equiv \mathbf{B}_{ai} \mathbf{C}_{bj}$ . Here  $\mathbf{L} \otimes \mathbf{L}$  is a sort of »super-matrix« which operates on the vector space of ordinary  $N \times N$  matrices, including  $\Omega$ . Then our equation can be written even more compactly as

$$(\mathbf{L} \otimes \mathbf{L})\Omega = 2\mathbf{L}$$

(where  $\Omega$  and  $\mathbf{L}$  on the right-hand side are understood to be here viewed as  $N^2 \times 1$  »super-vectors«). Now the super-matrix  $\mathbf{L} \otimes \mathbf{L}$  does not have a proper inverse, because it has 0-eigenvalue eigenvectors as follows from the null eigenvalue of  $\mathbf{L}$  (and because  $\mathbf{B} \otimes \mathbf{C}$  has eigenvalues which may be verified to be products of those of  $\mathbf{B}$  and  $\mathbf{C}$ ). But  $\mathbf{L} \otimes \mathbf{L}$  does have a generalized inverse  $\Gamma \otimes \Gamma$  which is zero on the null space of  $\mathbf{L} \otimes \mathbf{L}$ , and on the orthogonal subspace may be verified to multiply onto  $\mathbf{L} \otimes \mathbf{L}$  to give the identity (on this orthogonal

space). Thence the application of  $\Gamma \otimes \Gamma$  to the equation  $(\mathbb{L} \otimes \mathbb{L})\Omega = 2\mathbb{L}$  gives only the part of  $\Omega$  not in this null subspace – that is, it gives  $\Omega$  up to an additional correction in the null space. And this additional correction may be expressed as a sum of null eigenvectors to  $\mathbb{L} \otimes \mathbb{L}$ , such null eigenvectors being verified to be  $\varphi \otimes \beta$  and  $\alpha \otimes \varphi$  for arbitrary  $N$ -vectors  $\alpha$  and  $\beta$ . Thence the general solution for  $\Omega$  as dictated by the conditions of theorem  $D$  is

$$\Omega = 2 (\Gamma \otimes \Gamma)\mathbb{L} + \varphi \otimes \beta + \alpha \otimes \varphi$$

Now

$$((\Gamma \otimes \Gamma)\mathbb{L})_{ab} = \sum_{i,j} \Gamma_{ai} \Gamma_{bj} L_{ij} = (\Gamma \mathbb{L} \Gamma)_{ab} = \Gamma_{ab}$$

(where for the final equality it has been recalled that  $\mathbb{L}$  is symmetric in its indices). Thus this general solution is given in the form

$$\Omega_{ab} = 2 \Gamma_{ab} + \varphi_a \beta_b + \alpha_a \varphi_b = 2 \Gamma_{ab} + \beta_b + \alpha_a .$$

Next the symmetry condition ( $\Omega_{ab} = \Omega_{ba}$ ) leads to  $\beta_b + \alpha_b = \beta_a + \alpha_a$  and consequently  $\beta_b - \alpha_b = \beta_a - \alpha_a$ , independently of the choice of  $a$  and  $b$ . Thence this difference  $\beta_a - \alpha_a$  must in fact be independent of  $a$ , as we summarize by writing  $\beta_a - \alpha_a = 2\gamma$ . Next the condition of zero diagonal (for  $\Omega$ ) implies

$$0 = \Omega_{aa} = 2 \Gamma_{aa} + \beta_a + \alpha_a = 2 \Gamma_{aa} + 2\alpha_a + 2\gamma$$

so that  $\alpha_a = -\Gamma_{aa} - \gamma$ . Then also  $\beta_a = \alpha_a + 2\gamma = -\Gamma_{aa} + \gamma$ . Thus the final particular solution satisfying the symmetry and zero-diagonality conditions is

$$\Omega_{ab} = 2 \Gamma_{ab} - \Gamma_{bb} + \gamma - \Gamma_{aa} - \gamma = 2\Gamma_{ab} - \Gamma_{bb} - \Gamma_{aa}$$

which is the correct result, and the theorem is thereby established.

That is, the local conditions of theorem  $D$  have essentially all the information to determine the  $\Omega_{ij}$ . A question of interest is whether it is of a useful form. Actually going through the detailed inversion for  $\mathbb{L} \otimes \mathbb{L}$  in the proof of the theorem  $E$ , is certainly at least as difficult as going through the inversion for  $\mathbb{L}$  as indicated in theorem  $A$ . We come back to the utility of theorem  $D$  in the next section. Here it has been established that though we have considered a specific set of local sum rules in theorem  $D$ , the set is »complete«.

In contrast to the »local« sum rules of theorem  $D$ , one may choose  $\mathbb{M}$  to be a matrix which is a (matrix) graph invariant, with rows and columns which are labelled by vertices of  $G$ . Such sum rules are »global« and end up involving ordinary scalar graph invariants. Such choices for the matrix  $\mathbb{M}$  include  $\mathbb{A}$ ,  $\Delta$ ,  $\mathbb{L}$ ,  $\Gamma$ ,  $\mathbb{I}$  (the identity matrix),  $\mathbb{D}$  (the distance matrix for the

usual shortest-path metric), or various combinations of these matrices. Often such a choice leads to a relation between graph invariants involving the  $\Omega_{ij}$  and those seemingly not involving the  $\Omega_{ij}$ .

An example might be developed involving a particularly well-known graph invariant, namely, Randić's<sup>15</sup> so-called *connectivity index*

$${}^1\chi \equiv \sum_{\{i,j\} \in E} (\Delta_i \Delta_j)^{-1/2}.$$

Then if  $\mathbb{M}$  (in theorem *B*) is taken to be  $\Delta^{-1/2} \mathbb{A} \Delta^{-1/2} \equiv \overline{\mathbb{A}}$ , one finds

*Corollary F* – Let  $G$  be a connected graph with vertex and edge sets  $V$  and  $E$ . Then

$${}^1\chi = \sum_{\{i,j\} \in E} (\Delta_i \Delta_j)^{1/2} \Omega_{ij} - \sum_{k \in V} \sum_{\{i,j\} \subseteq n(k)} \frac{\Delta_i^{1/2} + \Delta_j^{1/2}}{\Delta_k^{1/2}} \Omega_{ij} + \sum_{\{i,j\} \in E} \sum_{k \in n(i)} \sum_{l \in n(j)} (\Delta_i \Delta_j)^{-1/2} \Omega_{ij}.$$

Though  ${}^1\chi$  has been extensively utilized<sup>15,16</sup> for structure/property and structure/activity correlations for a vast variety of molecules and properties (or activities), it seems that none of the three invariants on the right-hand side of the equation in this corollary have been previously contemplated. Another sum rule involving  ${}^1\chi$  occurs with the choice  $\mathbb{M} = \Gamma \overline{\mathbb{A}}$ , but again the  $\Omega$ -containing invariants that are then related to  ${}^1\chi$  seem to be previously unconsidered. Sum rules for higher order connectivity indices are also conceivable, as well as many other topological indices which have arisen in »chemical graph theory«. Substitutions for  $\mathbb{M}$  of a wide variety of standard ( $N \times N$ ) graph-theoretic matrices are possible – use of the shortest-path distance matrix  $\mathbb{D}$  or its powers, in particular would give sorts of inter-relations between the shortest-path and resistance distances. If  $s_i$  is defined as the sum of the shortest-path distances of the  $i$ th row of  $\mathbb{D}$  and  $\mathbb{S}$  is taken to be the diagonal matrix with these  $s_i$  along the diagonal, then  $\mathbb{M} = \mathbb{S}^{-1/2} \mathbb{A} \mathbb{S}^{-1/2}$  (or  $\mathbb{M} = \Gamma \mathbb{S}^{-1/2} \mathbb{A} \mathbb{S}^{-1/2}$ ) leads to a relation involving the Balaban<sup>17</sup> index  $J$  (in particular  $\text{tr}\{\mathbb{M}\mathbb{L}\}$  gives  $J$  up to a factor of  $e/(1 + \mu)$ , with  $e$  the number of edges and  $\mu$  the cyclomatic index). Evidently enormous numbers of yet other sum rules are possible. But typically the relations found by application of the theorem *B* seem to interrelate known indices to more than one new ( $\Omega$ -containing) »topological index«. What really might be desired is that all the graph invariants involved in more interesting inter-relations should have some independent motivation.

Here we focus on what might be perceived to be a »canonical« sequence of »global« sum rules, with that of corollary *C* being but the first member. Toward this end we introduce weighted sums over  $n$ -step walks between various vertices ( $i$  and  $j$ ) of  $G$ ,

$$w_{ij}(n) \equiv (\mathbb{A}(\Delta^{-1}\mathbb{A})^{n-1})_{ij}, \quad n \geq 1.$$

That is,  $w_{ij}(n)$  is a sum over  $n$ -step walks between vertices  $i$  and  $j$  with a weight which is a product of  $\Delta_{ii}^{-1}$  for each one of the internal vertices  $i$  of such a walk. It may be noted that  $w_{ij}(n)$  has a sort of probabilistic interpretation in terms of »random« walks. Such random walks passing through a vertex  $i$  in the walk take the next step along any one of the  $\Delta_i$  edges at  $i$  with equal probability. Thence,  $w_{ij}(n)/\Delta_i$  gives the probability  $p_n[j|i]$  that an  $n$ -step walk starting from site  $i$  ends at site  $j$  (and also  $p_n[i|j] = w_{ij}(n)/\Delta_j$ ). Thus  $w_{ij}(n)$  may be viewed to be the symmetric part of  $p[i|j]$  which is also common to  $p[j|i]$ . If one wished one could introduce  $n$ -step walk matrices  $\mathbb{W}(n)$  with elements  $w_{ij}(n)$ , and this would be reminiscent of the »walk matrices« introduced by Diudea<sup>18</sup> though his do not ordinarily seem to involve the  $\Delta_i^{-1}$  factors, such as relate to unbiased random walking (as we have noted). Sums over rather similarly weighted self-returning walks may also be defined

$$t_n \equiv \sum_{j \in V} w_{ii}(n)/\Delta_{ii}, \quad n \geq 1.$$

That is, this is just a trace over  $(\mathbb{A}\Delta^{-1})^n$ , or over the  $n$ th power of the symmetric matrix  $\Delta^{-1/2}\mathbb{A}\Delta^{-1/2} \equiv \overline{\mathbb{A}}$  (such being involved in an alternative<sup>11</sup> definition of the graph Laplacian, as  $\overline{\mathbb{L}} \equiv \mathbb{I} - \overline{\mathbb{A}}$ ). These  $t_n$  are graph invariants, with  $t_n/N$  being the probability that a random  $n$ -step walk be self-returning (presuming that each site  $i$  for initiation of the walk is equally likely). The sum-rules to be enunciated are for the invariants

$$S_n \equiv \frac{1}{2} \sum_{i,j \in V} w_{ij}(n) \Omega_{ij}, \quad n \geq 1.$$

Indeed we have:

*Theorem G* – For a connected  $N$ -site graph  $G$ ,

$$S_1 = N - 1, \quad S_2 = N - 2, \quad \text{and} \quad S_n = N - n + \sum_{i=2}^{n-1} t_i, \quad n \geq 3.$$

As a start for the proof, the result for  $S_1$  is involved in corollary *C*, which if translated into the current notation may be expressed as  $S_1 = N - 1$ . The result for  $S_2$  is derived from theorem *B* with the choice  $\mathbb{M} = \Delta^{-1}$ , which yields

$$\begin{aligned} 0 - 2S_1 + S_2 &= \frac{1}{2} \sum_{i,j \in V} (\Delta - 2\mathbb{A} + \mathbb{A}\Delta^{-1}\mathbb{A})_{ij} \Omega_{ij} = \frac{1}{2} \sum_{i,j \in V} (\mathbb{L}\Delta^{-1}\mathbb{L})_{ij} \Omega_{ij} = \\ &= -\text{tr}\{\Delta^{-1}\mathbb{L}\} = -\text{tr}\{\mathbb{I} - \Delta\mathbb{L}\} = -N \end{aligned}$$

and thence  $S_2 = N - 2$ , with the recognition that  $t_1 = 0$ . Now for the general case consider theorem *B* with  $\mathbb{M} = \Delta^{-1}(\mathbb{A}\Delta^{-1})^{n-1}$ , for  $n \geq 1$ , whence



$$S_{n+2} - 2S_{n+1} + S_n = \frac{1}{2} \sum_{i,j \in V} (L\Delta^{-1}(A\Delta^{-1})^{n-1} L)_{ij} \Omega_{ij} =$$

$$- \operatorname{tr}\{\Delta^{-1}(A\Delta^{-1})^{n-1} L\} = - \operatorname{tr}\{(\Delta\Delta^{-1})^{n-1} - \Delta^{-1}(A\Delta^{-1})^{n-1} A\} = - (t_{n-1} - t_n) .$$

But this is essentially a recursion relation for the resistance sums, and its use for  $n = 1$ , with the recognition that  $t_1 = 0$  and  $t_0 \equiv 0$ , then yields  $S_3 = N - 3 + t_2$ . Finally, use of mathematical induction then straight-forwardly completes the proof.

This thence indicates some sort of connection between resistance distances and random walks. Indeed such a connection in other contexts is known.<sup>8,19-22</sup>

### SPECIALIZED RESULTS FOR HIGHLY REGULAR GRAPHS

It turns out that both our »local« and »global« sum rules (of theorems *D* and *F*) rather readily determine some resistance distances for more highly regular graphs. Thence it is of relevance to refer to symmetry equivalence classes of pairs of vertices. The symmetry equivalence addressed here is that under the full *automorphism group*  $\mathcal{A}$  of the graph  $G$  – i.e.,  $\mathcal{A}$  is the set of vertex permutations which preserve edges. And the equivalence class containing a pair  $\{i,j\} \subseteq V$  is just the set of all pairs  $\{P(i), P(j)\}$  for  $P \in \mathcal{A}$ . Let  $\xi$  be a generic label for such a class, let  $\#_\xi$  denote the numbers of (unordered) pairs of such vertices, and let  $w_\xi(n)$  and  $\Omega_\xi$  denote the common values for  $w_{i,j}(n)$  and  $\Omega_{ij}$  for pairs  $\{i,j\}$  in this class. Then

$$S_n = \sum_{\xi} \#_{\xi} w_{\xi}(n) \Omega_{\xi} .$$

Only pairs  $\xi$  with an intersite distance  $\leq n$  occur in this sum, so that it may be quite limited, for sufficiently highly regular graphs. The pair with  $i = j$  does not occur in this sum (because  $\Omega_{ii} = 0$ ), but  $w_{ii}(n)$  is still defined though now the equivalence classes  $\eta$  are essentially those of a single site. Then denoting the degree of a site in such an equivalence class  $\eta$  as  $\Delta_\eta$ , the  $t_i$  may be reexpressed as

$$t_i = \sum_{\eta} \#_{\eta} w_{\eta}(i) / \Delta_{\eta} .$$

Overall the relation of theorem *F* may involve sums as in these symmetry-reduced expressions for  $S_n$  and  $t_i$  with rather few terms if the graph is sufficiently highly regular.

For a vertex transitive graph, there is just one orbit  $\eta$  ( $\equiv 0$ ) for individual sites, and for an edge transitive graph there is just one orbit  $\xi$  ( $\equiv 1$ ) for near-

est neighbor pairs of sites. Using either the  $S_1$  condition of theorem  $G$  or corollary  $C$  directly, one has:

*Corollary H* – For an edge transitive graph with  $N$  vertices and  $e$  edges, the nearest neighbor resistance distance is  $\Omega_1 = (N-1)/e$ .

This has been noted several times already.<sup>1,13,14,22</sup>

Vertex transitivity has important consequences for the self-returning walk probability sums

$$t_i = \#_0 w_0(i)/\Delta_0 = Nw_0(i)/\Delta_0$$

and there are consequences for the  $S_n$  also. In particular

*Theorem I* – Let  $G$  be an edge transitive connected graph, with  $c \in n(a)$ . Then

$$\sum_{i \in n(a)} \Omega_{ic} = 2\Delta_a \{(N-1)/e\} - 2.$$

The proof uses the  $a = b$  result of theorem  $D$ , and utilizes edge transitivity to change the sum over  $i \in n(a)$  to  $\Delta_a \Omega_1$ , and corollary  $H$  is used to substitute for  $\Omega_1$ . Then also the sum over  $\{i, j\} \in n(a)$  is noted to be equivalent to  $1/2$  times one over  $i, j \in n(a)$ , and then edge transitivity is used to eliminate one of these sums (say over  $j$  at a vertex  $c \in n(a)$ ).

Special cases of this theorem for graphs with additional regularity features (including vertex transitivity) have been noted.<sup>1,23</sup> With vertex transitivity also a result much like the result of corollary  $I$  may be obtained from the second ( $S_2$ ) part of theorem  $F$ .

The graphs of the regular polyhedra might be expected to lead to exceptionally simple results. These graphs have but one equivalence class for pairs of vertices at any given shortest-path distance  $d$ , so that the equivalence classes are naturally labelled by  $\xi \equiv d$ . The computation of the  $S_n$  entails counting different  $n$ -step walks between different pairs of vertices with different resistance distances therebetween. Then one finds that the condition for  $S_n$  may involve the  $\Omega_d$  for  $d$  up to  $n$ , and in application of the relations of theorem  $D$  in increasing order  $n$ , one finds a relation for  $\Omega_n$  in terms of those (already known)  $\Omega_d$  with  $d < n$ . That is, these relations of theorem  $D$  lead to a complete determination of all the resistance distances. In implementing this scheme, one finds the results of Table I. Here the results for the various  $\Omega_n$  agree with those of Lukovits *et al.*,<sup>24,25</sup> as corrected in Ref. 23. The results also agree with those of van Steenwijk.<sup>26</sup> The use of these global relation for  $S_n$  seems to become notably more tedious as  $n$  increases.

The graphs of the regular polyhedra may also be treated by corollary  $C$  and the local conditions of theorem  $D$ . Again one finds that as one proceeds

TABLE I

Invariants and resistance distances for global relations for the regular polyhedra

Polyhedron	$S_n$	$\Omega_n$
tetrahedron	$S_1 = 6 \cdot \Omega_1$	$\Omega_1 = 1/2$
octahedron	$S_1 = 12 \cdot \Omega_1$ $S_2 = 6 \cdot \Omega_1 + 3 \cdot \Omega_2$	$\Omega_1 = 5/12$ $\Omega_2 = 1/2$
cube	$S_1 = 12 \cdot \Omega_1$ $S_2 = 8 \cdot \Omega_2$ $S_3 = (28 \cdot \Omega_1 + 8 \cdot \Omega_3)/3 \left. \begin{array}{l} t_2 = 8/3 \end{array} \right\}$	$\Omega_1 = 7/12$ $\Omega_2 = 3/4$ $\Omega_3 = 5/6$
icosahedron	$S_1 = 30 \cdot \Omega_1$ $S_2 = 12 \cdot \Omega_1 + 12 \cdot \Omega_2$ $S_3 = (78 \cdot \Omega_1 + 48 \cdot \Omega_2 + 12 \cdot \Omega_3)/5 \left. \begin{array}{l} t_2 = 12/5 \end{array} \right\}$	$\Omega_1 = 11/30$ $\Omega_2 = 7/15$ $\Omega_3 = 1/2$
dodecahedron	$S_1 = 30 \cdot \Omega_1$ $S_2 = 20 \cdot \Omega_2$ $S_3 = 10 \cdot (5 \cdot \Omega_1 + 2 \cdot \Omega_2 + 2 \cdot \Omega_3)/3 \left. \begin{array}{l} t_2 = 20/3 \end{array} \right\}$ $S_4 = 20 \cdot (\Omega_1 + 7 \cdot \Omega_2 + 4 \cdot \Omega_3 + \Omega_4)/9 \left. \begin{array}{l} t_3 = 0 \end{array} \right\}$ $S_5 = 10 \cdot (29 \cdot \Omega_1 + 22 \cdot \Omega_2 + 22 \cdot \Omega_3 + 4 \cdot \Omega_4 + 2 \cdot \Omega_5)/27 \left. \begin{array}{l} t_4 = 5/27 \end{array} \right\}$	$\Omega_1 = 19/30$ $\Omega_2 = 9/10$ $\Omega_3 = 16/15$ $\Omega_4 = 17/15$ $\Omega_5 = 7/6$

to conditions for pairs of vertices at ever greater shortest-path distances, the relations involve  $\Omega_d$  for ever increasing values of  $d$ , and inversion to obtain the  $\Omega_d$  is relatively straight-forward. The relations resulting from theorem *D* are given in Table II. There the initial relations to determine  $\Omega_1$  are imagined to be the same as in Table I, so are not repeated again. And also reported in Table II is the sum  $W$  of all the resistances over all (unordered) pairs of vertices. This graph-invariant sum is an analogue of the Wiener number, and the values again agree with Palacios.<sup>23</sup> The use of the »local« relations for a pair of vertices ( $a$  and  $b$ ) at a distance  $n$  seems to become more tedious as  $n$  increases, though the tediousness seems to be a little less than for the corresponding global relation involving  $S_n$ .

An especially simple circumstance is found with the complete graph  $K_N$ , for which every pair of vertices have the same effective resistance,  $\Omega_1 = 2/N$ .

TABLE II  
Local relations and resistance sums for the regular polyhedra

Polyhedron	$\Omega_n$	$W'$
tetrahedron	$\Omega_1 = 3 \cdot \Omega_1 - 1$	2
octahedron	$(4\Omega_1 + 2 \cdot \Omega_2)/4 = 4 \cdot \Omega_1 - 1$	13/2
cube	$\Omega_2 = 3 \cdot \Omega_1 - 1$ $16 \cdot \Omega_1 + 2 \cdot \Omega_3 - 12 \cdot \Omega_2 = 2$	13
icosahedron	$\Omega_1 + \Omega_2 = 5 \cdot \Omega_1 - 1$ $18 \cdot \Omega_1 - 12 \cdot \Omega_2 + 2 \cdot \Omega_3 = 2$	28
dodecahedron	$\Omega_2 = 3 \cdot \Omega_1 - 1$ $14 \cdot \Omega_1 - 10 \cdot \Omega_2 + 2 \cdot \Omega_3 = 2$ $-5 \cdot \Omega_1 + 7 \cdot \Omega_2 - 4 \cdot \Omega_3 + \Omega_4 = 0$ $\Omega_1 - 4 \cdot \Omega_2 + 7 \cdot \Omega_3 - 5 \cdot \Omega_4 + \Omega_5 = 0$	548/3

The applicability of the theorematic results here even without vertex transitivity might be emphasized. For the complete bipartite graph (with  $m$  and  $n$  vertices in the two parts) corollary *H* directly yields

$$\Omega_1 = (m + n - 1)/mn, \quad G = K_{m,n}.$$

And letting  $\Omega_{2(m)}$  and  $\Omega_{2(n)}$  be the respective resistance distances between two vertices in the  $m$ - and  $n$ -site parts, the application of theorem *I* first for a site  $a$  in the  $n$ -site part and then for a site  $a$  in the  $m$ -site part leads to

$$\Omega_{2(m)} = 2/m \quad \text{and} \quad \Omega_{2(n)} = 2/n, \quad G = K_{m,n}.$$

Thereby all the resistance distances for the complete bipartite graph are obtained. It may be noted that if  $m$  and  $n$  are both large, then to a first approximation  $\Omega_1$  is just the average of  $\Omega_{2(m)}$  and  $\Omega_{2(n)}$ , so that amusingly the resistance distance between (one set of) next-nearest neighbor pairs of sites can be less than between nearest neighbors.

As yet another example the 14-site rhombic dodecahedron of Figure 1 might be considered. This has octahedral symmetry and may be viewed as the dual of the cubo-octahedron. From corollary *H* one finds  $\Omega_1 = 13/24$ , while from theorem *J* one may choose the primary vertex ( $a$  in the corollary) to be of degree 3 and then of degree 4, thereby obtaining

$$\Omega_{13} = 3 \Omega_1 - 1 = 5/8 \quad \text{and} \quad 2 \Omega_{24} + \Omega_{25} = 2(4 \Omega_1 - 1) = 7/3$$

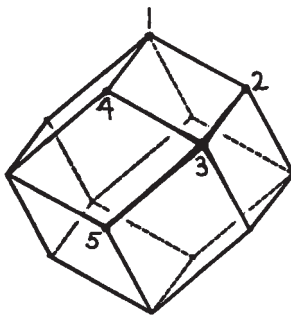


Figure 1. The rhombic dodecahedron, which is the dual of the cubo-octahedron.

where the vertex labelling is as in the figure. Two of these next nearest neighbor resistance distances thence are not determined, at this stage. For this polyhedron though there are 3 inequivalent sets of next nearest neighbors, it may be seen that there is but one class of next-next nearest neighbors, so that there is just one resistance distance  $\Omega_3$  for such pairs, and the next local sum rule of theorem *D* yields

$$12 \Omega_{21} - 8 \Omega_{13} - 3(2 \Omega_{24} + \Omega_{25}) + (9 \Omega_1 + 4 \Omega_3) = 2$$

whence  $\Omega_3 = 21/32$ .

The specialization of corollary *H* and theorem *I* to the limit of infinite lattice networks is of some interest. We have:

*Corollary J* – For infinite edge-transitive lattice networks, with  $c \in n(a)$ ,

$$\Omega_1 = 2/\bar{\Delta} \quad \text{and} \quad \sum_{i \in n(a)} \Omega_{ic} = 4(\Delta_c/\bar{\Delta}) - 2$$

where  $\bar{\Delta}$  is the average degree of the sites.

Notably these results apply whether or not the lattice is vertex transitive. With this extra assumption Thomassen<sup>27</sup> has established the first result for the limit of infinitely large lattice networks. For instance, for the rhomboidal lattice of Figure 2 one has twice as many degree 3 sites as degree 6 sites, so that  $\bar{\Delta} = (2/3) \cdot 3 + (1/3) \cdot 6 = 4$  and  $\Omega_1 = 1/2$ .

This corollary may be applied fairly readily for the example of all (four)<sup>28</sup> vertex- and edge-transitive 2-dimensional lattice networks. For the hexagonal lattice there is only one equivalent next-nearest neighbor pair, whence the sum rule (of corollary *J*) allows one to determine the corresponding resistance distance. However, for each of the remaining three example lattices there are two inequivalent next-nearest neighbor pairs.

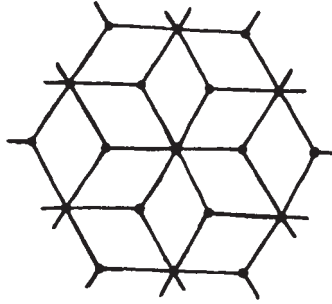


Figure 2. A section of the edge-transitive but not vertex-transitive rhomboidal lattice considered in the text.

For the hexagonal lattice:

$$\Omega_1 = 2/3 \text{ and } \Omega_2 = 1$$

where  $\Omega_2$  denotes the resistance distance between next nearest neighbors (all of which are equivalent).

For the square-planar lattice:

$$\Omega_1 = 1/2 \text{ and } 2 \Omega_2 + \Omega_{2'} = 2$$

where  $\Omega_2$  and  $\Omega_{2'}$  denote the respective resistances across the diagonal of a square and between two vertices separated 2 steps along either the  $x$ - or  $y$ -axes of the lattice.

For the triangular lattice:

$$\Omega_1 = 1/3 \text{ and } 6 \Omega_2 + 3 \Omega_{2'} = 4$$

where  $\Omega_2$  and  $\Omega_{2'}$  denote the respective resistances between two vertices across two triangles sharing a base and between two vertices separated 2 steps along any of the primitive translational lattice directions.

For the Kagome lattice:

$$\Omega_1 = 1/2 \text{ and } 6 \Omega_2 + 3 \Omega_{2'} = 4$$

where  $\Omega_2$  and  $\Omega_{2'}$  denote the respective resistances between two next-nearest neighbors within a hexagonal ring and between two vertices separated 2 steps along any of the primitive translational lattice directions.

Figure 3 shows small sections of these latter three lattices, and identifies pairs of vertices associated to  $\Omega_2$  and  $\Omega_{2'}$ . The behavior that the first lo-

cal sum rule determines a unique  $\Omega_2$  sometimes occurs for circumstances other than the hexagonal lattice – for instance, for the (tetrahedral) diamond lattice, one finds such an  $\Omega_2$  ( $= 2/3$ , while  $\Omega_1 = 1/2$ ).

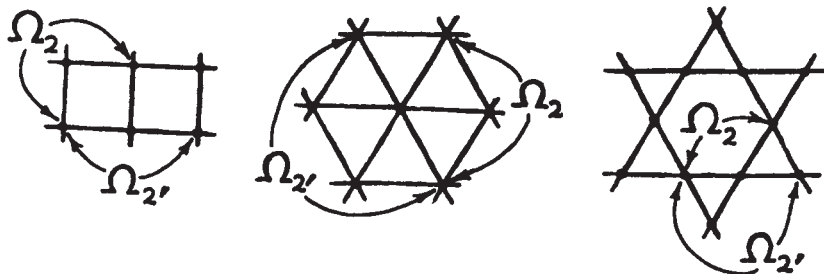


Figure 3. Small sections of the square-planar, triangular, and Kagome lattices, with an indication of the  $\Omega_2$  and  $\Omega_2'$  pairs of vertices in each case.

## CONCLUSION

Sum rules for resistance distances have been sought to be more thoroughly explored. A systematic complete sequence of »local« sum rules is found in theorem *D*. There are noted to be an endless variety of »global« sum rules which may also be viewed as inter-relations between a (possibly familiar) graph invariant without resistance distances and graph invariants involving resistance distances, though out of the vast variety many of the invariants seem typically to be quite »exotic«. A set of »global« sum rules are suggested to be »canonical« and thence are developed. This sequence of sum rules entails two sequences of graph invariants  $S_n$ ,  $n \geq 1$ , (involving the  $\Omega_{ij}$ ) and  $t_m$ ,  $m \geq 1$ , (not involving the  $\Omega_{ij}$ ). Each sequence involves random walking with the subscript ( $n$  or  $m$ ) identifying the number of steps in the random walks considered. Both the »local« and canonical »global« sum rules seem able to determine nearer neighbor resistance distances for sufficiently regular graphs, as is illustrated for several examples, including: the regular polyhedra; the 2-dimensional vertex- and edge-transitive lattice networks; the complete bipartite graph; and a few other cases. The first sum rule (of theorem *F* or corollary *C*) for the nearest neighbor resistance distances leads to particularly simple results for edge transitive graphs, and for more general circumstances the determination of next-nearest neighbor resistance sums seems most readily to proceed using the local sum rule of theorem *D*. It is here illustrated how the theorems may be used to determine re-

sistance distances for even more distant pairs of vertices. Thence further illuminating results are found for the resistance distance.

*Note added in proof:* Prof. J. L. Palacios points out that in Ref. 29 Foster established the  $S_2$  sum rule of Theorem G.

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## SAŽETAK

### Pravila sume otpornih udaljenosti

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Pošto su ukratko prikazane mogućnosti uporabe nove intrinzične grafovske metrike, otporne udaljenosti u kemiji, dan je niz pravila sume za tu metriku. Identificirana su »globalna« i »lokalna« pravila sume. Zbrojevi u »globalnim« pravilima sume grafovske su invarijante, a pravilo sume upućuje na međusobni odnos različitih invarijanti, od kojih neke uključuju otporne udaljenosti, a neke ne. Dane su ilustrativne primjene na gotovo »regularne« grafove.